

Accuracy of the WKB approximation: the case of general quartic potential

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We analyse the accuracy of the approximate WKB quantization for the case of general one-dimensional quartic potential. In particular, we are interested in the validity of semiclassically predicted energy eigenvalues when approaching the limit $E \rightarrow \infty$, and in the accuracy of low lying energy levels below the potential barrier in the case of generally asymmetric double-well quartic potential. In the latter case, using the standard WKB quantization an unnatural localization of eigenstates due to the negligence of tunneling is implied and thus the validity of semiclassics is uncertain. In all computations the higher order corrections to the leading semiclassical approximation are included using the complex contour integration technique. We show that these corrections can improve accuracy of semiclassical approximation greatly *by many orders of magnitude*.

§1. Introduction

The semiclassical approximation is a very useful approximative tool in quantum mechanics, not only because it often yields analytic expressions but also because it helps us to understand the correspondence between quantum features and classical mechanics, that is particularly important in the quantum chaos.

Certain rather naive thoughts about semiclassical approximation have been established in the past. Namely, it has been believed that the semiclassical quantization gives sufficiently accurate energy values of quantum eigenstates, when \hbar is sufficiently small, in comparison to some action that stands with it, and in the case of high energies as well. Both limits imply that the de Broglie wavelength must be sufficiently small, but they are nevertheless *not* equivalent unless the underlying Hamiltonian has the scaling property. But the crucial criterion for assessing the accuracy of semiclassically predicted energy values is the comparison of the absolute value of the error of semiclassical energies with the mean energy level spacing (Prosen and Robnik¹⁾). The fine structure, the statistical and other properties of energy spectra cannot be reliably resolved unless the error is small enough compared to the mean energy level spacing.

The usual semiclassical techniques like EBK quantization (Maslov²⁾) and Gutzwiller trace formula are just the first (leading) terms of a certain semiclassical expansion of quantum quantities in the \hbar power series. Typically these are only asymptotic series, but occasionally can nevertheless be convergent, as a surprise (see below). The absolute error of energies, predicted by those two methods is typically of order \hbar^2 ,

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while the mean energy level spacing scales as \hbar^f , where f is the number of degrees of freedom (dimension of the system's coordinate space). Thus, the two methods seem to be applicable only in systems whose dimensionality is less than three. At a fixed value of \hbar and in the limit of high energies $E \rightarrow \infty$, the situation is even worse. The error of the leading order semiclassical approximation, measured in the units of the mean energy level spacing, can diverge or is bounded from below as E goes to ∞ even in cases of one and two dimensional systems (Prosen and Robnik¹⁾, Robnik and Salasnich^{3), 4)}). Nevertheless, for some specific systems, all of them exactly solvable, the WKB series can be convergent and its sum equal to the exact result. See ref. ^{3), 4), 7) - 10)}.

In this paper we analyse a one-dimensional general quartic potential, for which we are able to calculate the systematic higher order correction in the \hbar expansion. Firstly we examine the simple case of pure quartic potential, also called homogeneous quartic oscillator, which is a scaling system, and thus we expect the $\hbar \rightarrow 0$ limit, to be equivalent to the $E \rightarrow \infty$ limit, so that the error of semiclassical energies in units of the mean energy level spacing should converge to zero as energy increases. Secondly, we tried to enrich our understanding of global behaviour of the semiclassical approximation by examining its validity in the case of potential with more than one minimum, like asymmetric double-well quartic potential. A standard semiclassical quantization condition, obtained by requiring that the complex wavefunction as a function of the complexified coordinate be singlevalued, demands that the change of the semiclassical phase around a circuit enclosing the two turning points (at the boundaries of the classically allowed regions) is an integer multiple of 2π . We assume that neglecting the tunneling, as an exponentially small effect, this quantization condition can be also used in the cases where classically allowed regions are separated in the coordinate space with the potential barrier. In these cases motion in each well is meant to be semiclassically quantized separately, and the error of energy values because of this unnatural localization is supposed to be exponentially small. Strictly speaking, we actually do not know rigorously how to interpret this quantization condition, which is another important reason to study the implementation of WKB methods and to test them in multi-well potentials like in our present work (also see Robnik and Romanovski⁹⁾). However, if one is interested explicitly in the fine structure of energy spectra, especially and in particular the exponentially small splitting (due to tunneling) in *symmetric* double well potentials, then the approach expounded in Robnik *et al*⁵⁾ is the appropriate one.

We show that the homogeneous and asymmetric nonhomogeneous quartic potential is indeed an example of a potential where the semiclassical approximation works well in all energy ranges that we were interested in. By adding higher order corrections, the accuracy of semiclassically predicted energy values measured in units of the mean energy level spacing can be increased by many orders of magnitude.

§2. Homogeneous quartic potential and semiclassical methods

The Hamiltonian of the simple homogeneous quartic potential, that we consider in this section is

$$H = \frac{p^2}{2m} + Ax^4 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + Ax^4. \quad (2.1)$$

Introducing the new scaled and dimensionless variables

$$\tilde{x} = x \left(\frac{mA}{\hbar^2} \right)^{1/6}, \quad \tilde{E} = E \left(\frac{m^2}{\hbar^4 A} \right)^{1/3}, \quad \tilde{\hbar} = 1, \quad (2.2)$$

the Hamiltonian can be rewritten in the simple form

$$\tilde{H} = -\frac{1}{2} \frac{\partial^2}{\partial \tilde{x}^2} + \tilde{x}^4. \quad (2.3)$$

In all further calculations only the scaled form of the Hamiltonian and of the variables will be used, so that the tilde will be omitted in the further writing. Note that the scaled energy is the only one system parameter.

We study this system for two main purposes. Namely, we are interested in the asymptotic ($E \rightarrow \infty$) behaviour of standard semiclassical quantization formulas of finite order in the case of scaling system like this, and further we want to compare the spectral properties of homogeneous quartic potential with the spectral properties of general asymmetric double well quartic potential which we also call non-trivial potential. Again, in this comparison we are mainly interested in the asymptotic properties meaning high energy behaviour of the spectrum of a non-trivial potential whose geometry is asymptotically the same (as $|x| \rightarrow \infty$) as for the homogeneous quartic potential. For these reasons we use the standard WKB quantization procedure rather than the implicit semiclassical formulas of Voros⁶).

To calculate the semiclassical spectrum of a Hamiltonian we observe that the wavefunction can always be written in the form

$$\psi(x) = \exp \left(\frac{i}{\hbar} \sigma(x) \right), \quad (2.4)$$

where $\sigma(x)$ is the complex phase that satisfies the Riccati differential equation (for σ')

$$\sigma'^2(x) + \frac{\hbar}{i} \sigma''(x) = 2m(E - V(x)). \quad (2.5)$$

The WKB approximation rests upon the expansion of the phase in the \hbar power series

$$\sigma(x) = \sum_{k=0}^{\infty} \left(\frac{\hbar}{i} \right)^k \sigma_k(x). \quad (2.6)$$

Substituting (2.6) into (2.5) and comparing like powers of \hbar gives the recursion relation for $\sigma'_k(x)$ ($n > 0$)

$$\sigma_0'^2 = 2m(E - V(x)), \quad \sum_{k=0}^n \sigma'_k \sigma'_{n-k} + \sigma''_{n-1} = 0. \quad (2.7)$$

The quantization condition is obtained by requiring that the complex wavefunction (2.4) is singlevalued as a function of the complexified coordinate, which means that the change of phase, when going around the classically allowed region between the two turning points a ($V(a) = E$) and b ($V(b) = E$), should be equal to an integer multiple of $2\pi\hbar$

$$\oint d\sigma = \sum_{k=0}^{\infty} \left(\frac{\hbar}{i}\right)^k \oint d\sigma_k = 2\pi\hbar n. \quad (2.8)$$

The integer n is the quantum number. The zeroth and the first order terms give the EBK or torus quantization formula, where the first order term gives the Maslov corrections with Maslov index 2 for one dimensional system. We observe that all the other odd terms in (2.8) vanish when integrated along the closed contour around the pair of turning points, because they are exact differentials which is a highly plausible hypothesis yet to be proved rigorously (Bender *et al*⁷⁾, Robnik and Romanovski⁹⁾) but it has been demonstrated to hold for some low orders. We should stress that the closed contour is the contour in the complex x plane, since all integrals in (2.8), except the zeroth order term, diverge when integrated on an interval along real x -axes between the two turning points (Bender *et al*⁷⁾, Robnik *et al*⁵⁾). However, there is a way of expressing these integrals as a partial derivative w.r.t. the energy of a fundamental real integral on the interval between the two turning points. Finally, taking this into account, the semiclassical quantization condition can be written as

$$\sum_{k=0}^{\infty} \left(\frac{\hbar}{i}\right)^{2k} \oint d\sigma_{2k} = 2\pi\hbar \left(n + \frac{1}{2}\right), \quad (2.9)$$

that is the sum over even-numbered terms only. The first three terms in (2.9) are

$$\oint d\sigma_0 = 2\sqrt{2m} \int_a^b \sqrt{E - V(x)} dx, \quad V(a) = V(b) = E, \quad (2.10)$$

$$\oint d\sigma_2 = \frac{1}{12\sqrt{2m}} \frac{\partial}{\partial E} \int_a^b \frac{V''(x)}{\sqrt{E - V(x)}} dx, \quad (2.11)$$

$$\oint d\sigma_4 = \frac{1}{576\sqrt{2m^3}} \left[\frac{7}{5} \frac{\partial^3}{\partial E^3} \int_a^b \frac{V''^2(x)}{\sqrt{E - V(x)}} dx - \frac{\partial^2}{\partial E^2} \int_a^b \frac{V''''(x)}{\sqrt{E - V(x)}} dx \right]. \quad (2.12)$$

A straightforward calculation of these terms for the case of the homogeneous quartic potential gives the semiclassical quantization formula with corrections up to the fourth order

$$E^{3/4} \sum_{k=0}^{k=2} a_k E^{-3k/2} = \pi \left(n + \frac{1}{2}\right);$$

$$a_0 = \frac{\Gamma\left(\frac{1}{4}\right)^2}{3\sqrt{\pi}}, \quad a_1 = -\frac{\pi\sqrt{\pi}}{4\Gamma\left(\frac{1}{4}\right)^2}, \quad a_2 = \frac{11\Gamma\left(\frac{1}{4}\right)^2}{6144\sqrt{\pi}}. \quad (2.13)$$

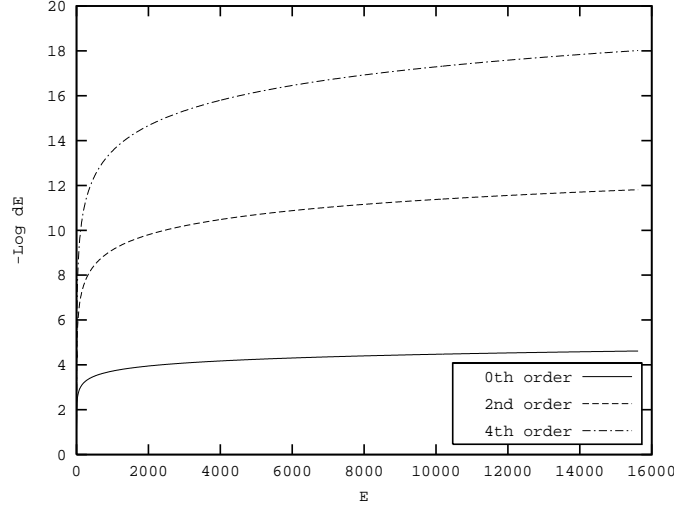


Fig. 1. The error of the 1100 lowest semiclassically predicted eigenenergies of the homogeneous quartic potential (HQP). Negative decadic logarithm of the error in units of mean energy level spacing ($-\text{Log } dE$) is plotted against energy E . The nearest level spacing is averaged over 7 nearest states to obtain the mean energy level spacing.

The exact spectrum is obtained by numerical diagonalization in QUADRUPLE PRECISION (32 valid digits) of the Hamiltonian matrix in the basis of eigenstates of harmonic oscillator, whose Hamiltonian is

$$H = \frac{1}{2}(\hat{p}^2 + \omega^2 x^2).$$

The matrix elements in this basis are

$$\begin{aligned} H_{n,m} = & \left(\frac{\omega}{4}(2n+1) + \frac{3}{4\omega^2}(2n^2+2n+1) \right) \delta_{n,m} + \\ & + \sqrt{(n+1)(n+2)} \left(-\frac{\omega}{4} + \frac{1}{2\omega^2}(2n+3) \right) \delta_{n+2,m} + \\ & + \sqrt{(n+1)(n+2)(n+3)(n+4)} \frac{1}{4\omega^2} \delta_{n+4,m}. \end{aligned} \quad (2.14)$$

The results of our calculations are plotted in the figure 1, where the negative decadic logarithm of the error of the semiclassical energies obtained from the zeroth order, the second order and the fourth order semiclassical quantization formula in units of the mean energy level spacing is plotted against energy. In table I of the Appendix B we show the numerical values for some representative energy levels, showing the fast increase in accuracy with higher orders of the semiclassical approximation.

From the plots we can deduce that the error really goes towards zero as we go to the high quantum numbers and/or energies. The accuracy of the semiclassics can be vastly enhanced, when higher order corrections in \hbar expansion are added to the EBK or torus quantization. Contrary to the case of potential $U_0/\cos^2(\alpha x)$ previously

studied (Prosen and Robnik¹⁾, Robnik and Salasnich³⁾), the homogeneous quartic potential is the case, where the $\hbar \rightarrow 0$ limit is equivalent to the $E \rightarrow \infty$ limit as we predicted in the introduction, due to the scaling properties of our system.

§3. Asymmetric double-well quartic potential

The Hamiltonian of the system that we consider in this section is generally written as

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + Ax^4 + Cx^3 - 2Bx^2. \quad (3.1)$$

Again we introduce the scaled variables

$$\tilde{x} = x\sqrt{\frac{A}{B}}, \quad \tilde{E} = E\frac{A}{B^2}, \quad \lambda = \frac{C}{\sqrt{AB}}, \quad \hbar_{eff} = \hbar\frac{A}{\sqrt{mB^3}}, \quad (3.2)$$

and rewrite the Hamiltonian containing these variables

$$H = -\frac{\hbar_{eff}^2}{2} \frac{\partial^2}{\partial x^2} + x^4 + \lambda x^3 - 2x^2. \quad (3.3)$$

The notation with tilde has already been omitted in the equation (3.3). The \hbar_{eff} and λ are two additional parameters of the asymmetric double-well quartic potential. The latter is called the parameter of asymmetry. To check the accuracy of the semiclassical quantization for this type of the system, we perform the semiclassical quantization separately for states with energy below the potential barrier ($E < 0$), and for the states with energy above the potential barrier ($E > 0$).

Neglecting the tunneling, those states below the potential barrier, are semiclassically quantized using the standard semiclassical procedure, described in the previous section, for both wells separately. We assume that the error committed by this approximation and localization is only exponentially small, since the tunneling is only exponentially small.

The calculation of the integrals (2.10), (2.11) and (2.12) that enter the semiclassical quantization formula (2.9) is much more complicated here than for the system discussed in the previous section. The expressions obtained immediately after the integration on coordinate x in (2.11) and (2.12) are very complex functions of the four roots of the momentum p , and energy. These functions should be further differentiated with respect to energy E . Please note, that the roots of $p = \sqrt{2(E - V(x))}$ are also dependent on energy and in case of the fourth order correction formula (2.12) a three-fold differentiation with respect to E should be done. The expression for the fourth order

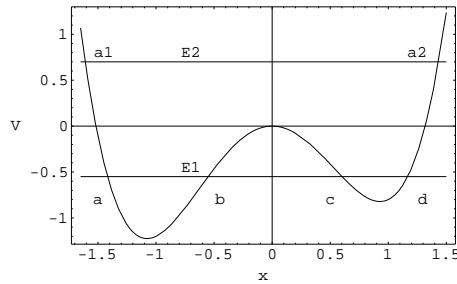


Fig. 2. A sketch of the asymmetric double-well quartic potential (ADWP)

corrections is thus too complex to be handled with our hardware equipment, regardless of the fact that we do not need to know the explicit dependence on E for the roots. The derivative of a root a with respect to the energy could be written in a form $da/dE = (dV(x)/dx)^{-1}|_{x=a}$. In most of the manipulations we used the *Mathematica* software. The calculation of expressions (2.10) and (2.11) are briefly sketched in the appendix A.

We have performed our calculations for three chosen values of \hbar_{eff} , namely at $\hbar_{eff} = 0.01$, $\hbar_{eff} = 0.1$ and $\hbar_{eff} = 1$, and at a fixed value of the parameter of asymmetry $\lambda = 0.2$. The shape of our asymmetric double well potential is shown in figure 2. The negative decadic logarithm of the error of the energies calculated with the zeroth order and the second order semiclassical quantization formula, in units of the mean energy level spacing, is plotted in the figures 3 and 4.

As we see from figures 3, 4 and from the table II in the appendix B, the accuracy of semiclassical methods increases with energy like in the homogeneous case. The accuracy is about 4 orders in magnitude or more greater when the second order corrections are included in the semiclassical quantization formula.

It is quite surprising how accurate the semiclassical quantization is even in the range of the energies below the potential barrier whilst close to the top of the barrier it is not so good, as expected. Of course we expect that the semiclassical methods are valid where the potential is similar to the harmonic potential and our expectation seems to be proved now. As we see the accuracy decreases and the improvement of the semiclassically predicted energies by considering the higher order semiclassical corrections e.g. σ_2 gets smaller as we approach the top of the barrier. This is expected, since the exponentially small error caused by the negligence of tunneling increases with energy, as we have shown in our previous work (Robnik *et al*⁵⁾). Our results of this section are depicted in figures 4-6. Generally, the accuracy of semiclassics increases as we decrease the value of \hbar_{eff} , what is of course expected and shown in figure 6.

Again, the exact spectrum has been calculated by numerical diagonalization in QUADRUPLE PRECISION of the Hamiltonian matrix in the basis of eigenstates of the harmonic oscillator. Because the symmetry w.r.t. parity operation is broken here, the matrix does not decompose into even and odd part any more. The matrix elements of the matrix in the same harmonic oscillator

$$H = \frac{1}{2}(\hat{p}^2 + \omega^2 x^2),$$

basis as before read as

$$\begin{aligned} H_{n,m} = & \left(\hbar_{eff} \left[\frac{\omega}{4} - \frac{1}{\omega} \right] (2n+1) + \frac{3\hbar_{eff}^2}{4\omega^2} (2n^2 + 2n + 1) \right) \delta_{n,m} + \\ & + 3\lambda \sqrt{\left[\frac{\hbar_{eff}}{2\omega} \right]^3} \sqrt{(n+1)^3} \delta_{n+1,m} + \\ & + \sqrt{(n+1)(n+2)} \left(-\hbar_{eff} \left[\frac{\omega}{4} + \frac{1}{\omega} \right] + \frac{\hbar_{eff}^2}{2\omega^2} (2n+3) \right) \delta_{n+2,m} + \end{aligned}$$

$$\begin{aligned}
& + \lambda \sqrt{\left[\frac{\hbar_{eff}}{2\omega}\right]^3} \sqrt{(n+1)(n+2)(n+3)} \delta_{n+3,m} + \\
& + \sqrt{(n+1)(n+2)(n+3)(n+4)} \frac{\hbar_{eff}^2}{4\omega^2} \delta_{n+4,m}.
\end{aligned} \tag{3.4}$$

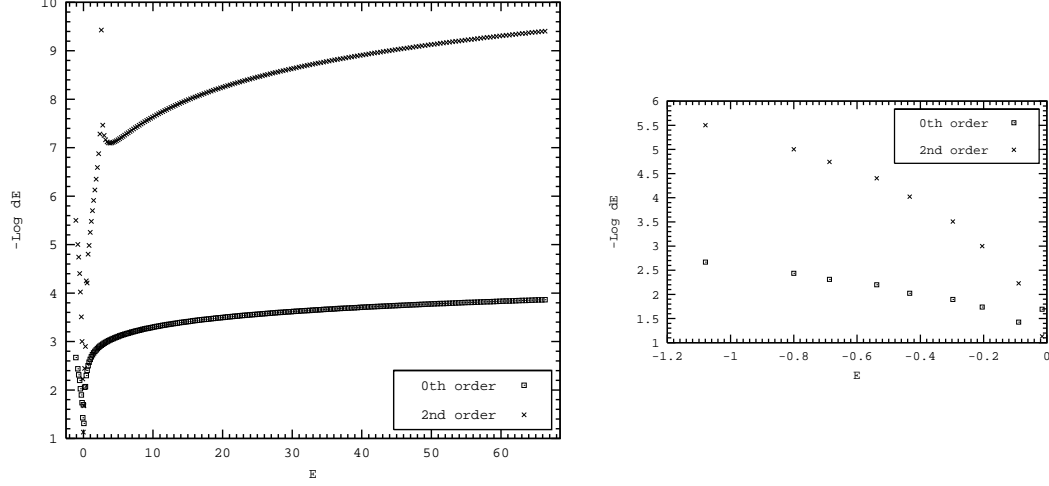


Fig. 3. Negative decadic logarithm of the error of the semiclassical energies in units of the mean energy level spacing ($-\text{Log } dE$) *vs.* energy (E) of 200 lowest states (left), of which 9 lie below the barrier and are separately plotted in the right graph. Asymmetric double-well quartic potential with $\hbar_{eff} = 0.1$ and $\lambda = 0.2$.

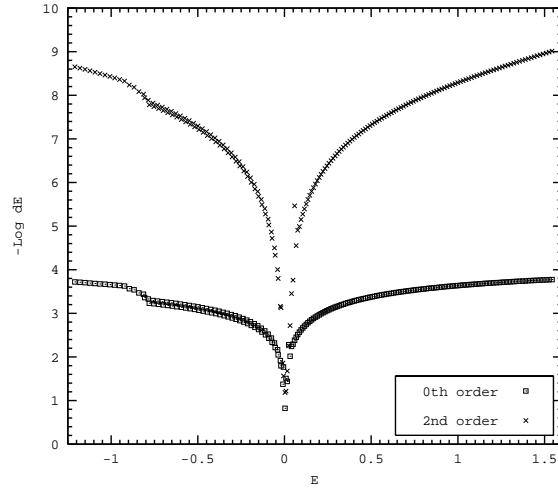


Fig. 4. Negative decadic logarithm of the error of the semiclassical energies in units of the mean energy level spacing ($-\text{Log } dE$) *vs.* energy (E) of 200 lowest states, of which 86 lie below the barrier. Asymmetric double-well quartic potential with $\hbar_{eff} = 0.01$ and $\lambda = 0.2$.

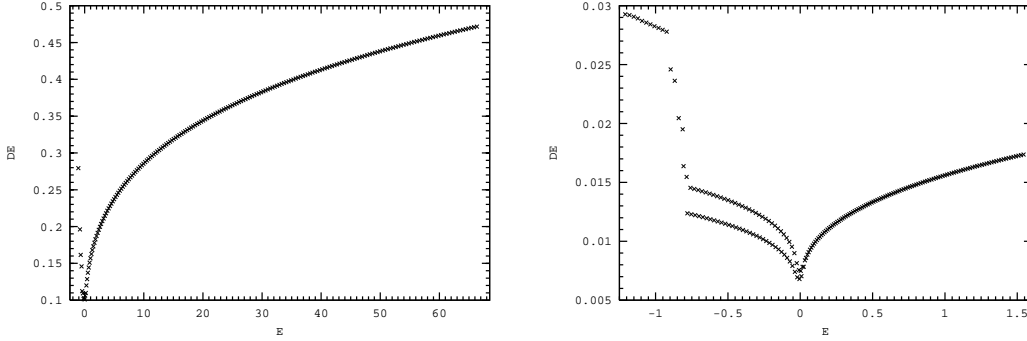


Fig. 5. The mean energy level spacing (DE), averaged over 7 nearest states, *vs.* energy (E) of 200 lowest states. Asymmetric double-well quartic potential with $\hbar_{eff} = 0.1$ and $\lambda = 0.2$ (left) and $\hbar_{eff} = 0.01$ and $\lambda = 0.2$ (right).

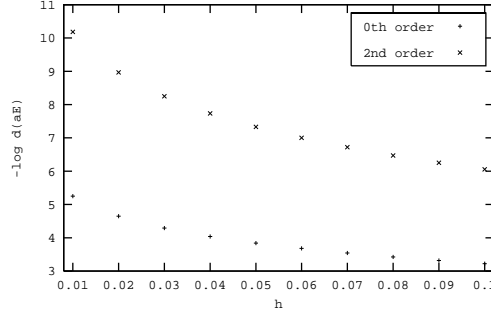


Fig. 6. Negative decadic logarithm of the absolute error of the semiclassical energies of the ground state ($-\text{Log } d(aE)$) *vs.* \hbar_{eff} (h). Asymmetric double-well quartic potential with $\lambda = 0.2$.

§4. High energy correspondence between the exact spectra of the homogeneous and the general quartic potential

During our work new questions about the spectral properties of the systems with non-trivial potential have arisen. By the word non-trivial potential we mean e.g. the asymmetric double-well quartic potential and similar potentials with complicated structure in certain regions of coordinate space and with a simple asymptotic behaviour as $|x| \rightarrow \infty$. The question is, whether the spectra of the homogeneous quartic potential and that of the asymmetric double-well potential with $\hbar = 1$ converge pointwise or at least to a certain shift in energy and in the quantum number, as $E \rightarrow \infty$.

The scaled Hamiltonian of the general quartic potential can be written as

$$H = \frac{p^2}{2} + x^4 + \mu V_1(x)$$

$$V_1(x) = \lambda x^3 - 2x^2. \quad (4.1)$$

In the following figures we present the comparison of the spectrum for the case $\mu = 0$ with the spectrum of the system where $\mu = 1$, $\lambda = 0.2$. We compare about 500 lowest states. In the figures 7 the mean energy level spacing against energy is plotted for both systems. The discrepancy between the curves for the two systems is clearly seen. To any state of $\mu = 0$ case we find the state of $\mu = 1$ case which is energetically most close to it and in figure 8 we plot the discrepancy of those energies measured in the units of the mean energy level spacing of the $\mu = 0$ case, against the energy of $\mu = 0$ states. We clearly see some cut-offs that occur at some energy values, where the difference in quantum numbers of the energetically nearest states of the two systems is enlarged by 1.

To understand these features we calculate the zeroth order semiclassical approximation for the mean energy level spacing DE (the Thomas-Fermi formula).

$$DE_{ADWP} = \frac{dE}{dn} = \pi \left[\int_{a_1}^{a_2} \frac{dx}{p(x)} \right]^{-1}, \quad p = \sqrt{2(E - V(x))}, \quad p(a_1) = p(a_2) = 0. \quad (4.2)$$

For the case of the asymmetric double well potential (ADWP) the integral in the expression above becomes

$$\int_{a_1}^{a_2} \frac{dx}{\sqrt{E - V(x)}} = \frac{2}{\sqrt{kq}} \mathbf{F}(m) \quad (4.3)$$

$$k^2 = (a_1 - b)^2 + c^2, \quad q^2 = (a_2 - b)^2 + c^2, \quad m = \frac{kq - (a_1 - b)(a_2 - b) - c^2}{2kq},$$

where b and $\pm c$ are the real and the imaginary part of the other two complex conjugate roots of $p(x)$ (see appendix A). To calculate the mean energy level spacing for the ADWP case we expand the 4 roots of $E - V(x)$ into the energy E asymptotic series. The first few terms of those series are

$$a_{1,2} = \mp E^{1/4} - \frac{\lambda\mu}{4} \mp \left[\frac{3(\lambda\mu)^2}{32} + \frac{\mu}{2} \right] E^{-1/4} - \lambda\mu \left[\frac{(\lambda\mu)^2}{32} + \frac{\mu}{4} \right] E^{-1/2} \\ \mp \frac{15(\lambda\mu)^4 + 160(\lambda\mu)^2\mu + 256\mu^2}{2048} E^{-3/4} + O(E^{-5/4}), \quad (4.4)$$

$$b \pm ic = -\frac{\lambda\mu}{4} + \lambda\mu \left[\frac{(\lambda\mu)^2}{32} + \frac{\mu}{4} \right] E^{-1/2} + i \left\{ E^{1/4} - \left[\frac{3(\lambda\mu)^2}{32} + \frac{\mu}{2} \right] E^{-1/4} \right\} \\ + i \left\{ \frac{15(\lambda\mu)^4 + 160(\lambda\mu)^2\mu + 256\mu^2}{2048} E^{-3/4} \right\} + O(E^{-5/4}). \quad (4.5)$$

Now, we can do the same with the quantities $2/\sqrt{kq}$ and m

$$\frac{2}{\sqrt{kq}} = \sqrt{2}E^{-1/4} - \frac{3(\lambda\mu)^4 + 32(\lambda\mu)^2\mu + 64\mu^2}{128\sqrt{2}} E^{-5/4} + O(E^{-7/4}), \quad (4.6)$$

$$m = \frac{1}{2} + \left[\frac{3(\lambda\mu)^2}{32} + \frac{\mu}{2} \right] E^{-1/2} + O(E^{-3/2}) . \quad (4.7)$$

Bearing in mind that

$$\frac{\partial \mathbf{F}(m)}{\partial m} = \frac{1}{2m(1-m)} (\mathbf{E}(m) - (1-m)\mathbf{F}(m)) \quad (4.8)$$

we expand the elliptic integral $\mathbf{F}(m)$ into the asymptotic series around $m = 1/2$. Rewriting

$$\mathbf{F}(1/2) = \frac{\Gamma(1/4)^2}{4\sqrt{\pi}} \quad (4.9)$$

and

$$\mathbf{E}(1/2) = \frac{\Gamma(1/4)^2}{8\sqrt{\pi}} \left(1 + \frac{8\pi^2}{\Gamma(1/4)^4} \right) , \quad (4.10)$$

finally we get an asymptotic expression for the mean energy level spacing

$$DE_{ADWP} = E^{1/4} \frac{4\sqrt{\pi}^3}{\Gamma(1/4)^2} \left[1 - E^{-1/2} \frac{\pi^2}{4\Gamma(1/4)^4} (16\mu + 3(\lambda\mu)^2) \right] . \quad (4.11)$$

It is easy to see that the factor outside the brackets is just the mean energy level spacing of the homogeneous quartic potential (HQP)

$$DE_{HQP} = E^{1/4} \frac{4\sqrt{\pi}^3}{\Gamma(1/4)^2} . \quad (4.12)$$

The zeroth order semiclassical predictions for the mean energy level spacing (4.11) and (4.12) are also plotted in figures 7. The result (4.11) can be obtained also perturbatively by a systematic perturbative treatment of the integral (4.2).

Further we analyze the difference D of energetically nearest states of HQP and ADWP in units of mean energy level spacing of HQP. For this purpose we expand the zeroth order semiclassical quantization condition for ADWP

$$\begin{aligned} \int_{a_1}^{a_2} p dx &= \frac{4\sqrt{2}}{3} \frac{1}{\sqrt{kq}} \left\{ \left[E - \frac{(\lambda\mu)\mu}{4} \frac{a_2 k - a_1 q}{k - q} + \left(\mu + \frac{3(\lambda\mu)^2}{16} \right) \frac{a_2^2 k - a_1^2 q}{k - q} \right] \mathbf{F}(m) + \right. \\ &\quad \left. + \left(\mu + \frac{3(\lambda\mu)^2}{16} \right) kq \mathbf{E}(m) + \right. \\ &\quad \left. + \frac{3\lambda\mu}{8} \left(\mu + \frac{(\lambda\mu)^2}{8} \right) \frac{(a_2 - a_1)(k + q)}{k - q} \mathbf{\Pi}(n, m) \right\} = \pi \left(M + \frac{1}{2} \right) ; \quad n = -\frac{(k - q)^2}{4kq} \end{aligned} \quad (4.13)$$

(see the end of the appendix A) into the asymptotic energy series, valid at high energies. To do that we follow the similar procedure as in the case of derivation of the mean energy level spacing asymptotic expression (4.11). Here we also use the first order expansion of the three elliptic integrals for small arguments ϵ and δ

$$\mathbf{F}(1/2 + \epsilon) = \mathbf{F}(1/2) + (2\mathbf{E}(1/2) - \mathbf{F}(1/2))\epsilon ,$$

$$\begin{aligned}\mathbf{E}(1/2 + \epsilon) &= \mathbf{E}(1/2) + (\mathbf{E}(1/2) - \mathbf{F}(1/2))\epsilon, \\ \mathbf{II}(0 + \delta, 1/2 + \epsilon) &= \mathbf{F}(1/2) + (2\mathbf{E}(1/2) - \mathbf{F}(1/2))\epsilon + 2(\mathbf{F}(1/2) - \mathbf{E}(1/2))\delta,\end{aligned}$$

in our case

$$\epsilon = m - \frac{1}{2} = \left[\frac{3(\lambda\mu)^2}{32} + \frac{\mu}{2} \right] E^{-1/2} + O(E^{-3/2}), \quad \delta = n = O(E^{-3/2})$$

and so we get an asymptotic expression of the condition (4.13)

$$\pi \left(M + \frac{1}{2} \right) = E^{3/4} \frac{\Gamma(1/4)^2}{3\sqrt{\pi}} \left[1 + E^{-1/2} \frac{3\pi^2}{4\Gamma(1/4)^4} (16\mu + 3(\lambda\mu)^2) \right] + O(E^{-1/4}). \quad (4.14)$$

Note, that the leading term of the upper equation (4.14) is precisely the zeroth order semiclassical quantization condition for HQP (see (2.13))

$$\pi \left(N + \frac{1}{2} \right) = E^{3/4} \frac{\Gamma(1/4)^2}{3\sqrt{\pi}}. \quad (4.15)$$

Since the M -th energy eigenvalue $E + \Delta E$ of ADWP is energetically nearest to the N -th eigenenergy E of the HQP (by definition ΔE is smaller than one half of the mean energy level spacing), we expand the difference of equations (4.14) and (4.15) into the $\Delta E/E$ power series up to the first order and solve it for ΔE . Finally we can write an approximate expression for the energy difference of the energetically closest states of ADWP and HQP at high energies

$$\Delta E = DE_{AQWP} \left[(M - N) - \frac{\sqrt{\pi}}{4\Gamma(1/4)^2} (16\mu + 3(\lambda\mu)^2) E^{1/4} \right], \quad (4.16)$$

of which the leading term in the units of mean energy level spacing of HQP is

$$D = \frac{\Delta E}{DE_{HQP}} \approx (M - N) - \frac{\sqrt{\pi}}{4\Gamma(1/4)^2} (16\mu + 3(\lambda\mu)^2) E^{1/4}. \quad (4.17)$$

The above expression is also plotted in the figure 8 together with the exact results.

According to the expression (4.17) and also with respect to the exact results, plotted in figure 8 we can conclude that the two spectra do not converge pointwise and not even converge to a constant energy shift since the expression (4.17) as a function of energy never reaches the constant value of D at a fixed value of difference between the appropriate quantum numbers N and M of the homogeneous quartic potential and the asymmetric double well potential.

The expression (4.11) that fits the exact data quite well indicates that the mean energy level spacing of the asymmetric double well potential converges to the mean energy level spacing of HQP as energy increases but it converges as slow as $E^{-1/4}$.

§5. Conclusions

According to our results we can conclude that the semiclassical approximation gives sufficiently good results in the case of the quartic potential. As we see the

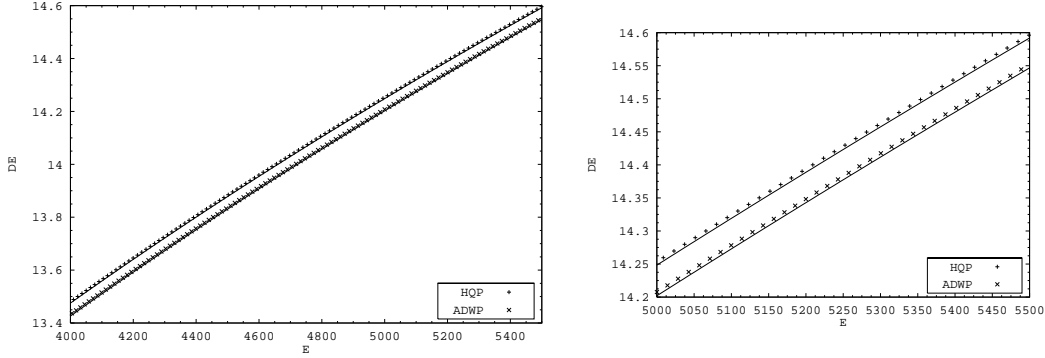


Fig. 7. Mean energy level spacing DE *vs.* energy E of the states between 400th and 500th state of HQP and ADWP ($\mu = 1$, $\lambda = 0.2$) (left). The right figure shows an enlarged window of the left figure at the energy range $[5000, 5500]$. Solid line is the zeroth order semiclassical prediction (Thomas-Fermi rule).

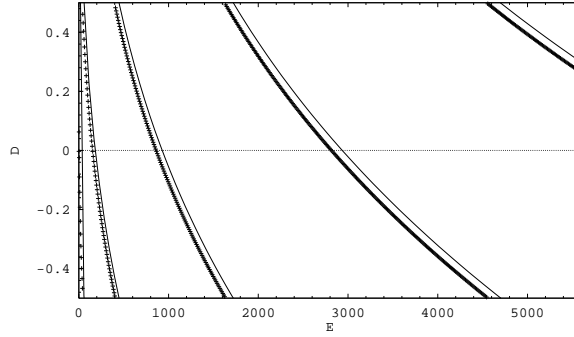


Fig. 8. Energy difference of energetically nearest states of $\mu = 0$ case (HQP) and $\mu = 1$, $\lambda = 0.2$ case (ADWP) *vs.* energy E of about 500 lowest states of HQP. The difference or discrepancy D is measured in units of mean energy level spacing of the HQP. Solid line is the zeroth order semiclassical prediction.

semiclassical energies in units of the mean energy level spacing converge to the exact ones for the case of homogeneous quartic potential as $E \rightarrow \infty$. Due to this scaling properties of the system we can talk about only one limit in this particular system where the semiclassics becomes exact, namely the semiclassical limit which is equivalent to the $\hbar \rightarrow 0$ or $E \rightarrow \infty$ limit. The accuracy of the semiclassical energies at the high energy values is not spoiled even in the case of asymmetric double-well quartic potential, which is not a scaling system. Even in the energy range below the potential barrier the accuracy of the semiclassics is very good, and it is bounded with the exponential error due to the negligence of tunneling. It is encouraging that the higher order corrections in the \hbar expansion of the semiclassical quantization formula increase the accuracy by many orders of magnitude. Obviously, the corrections like these are needed in two or more dimensional systems to prevent the error to diverge or to be bounded from below as we approach $\hbar \rightarrow 0$ or $E \rightarrow \infty$ limit. Some

recent related papers are Robnik and Salasnich^{3), 4)}, Robnik and Romanovski^{8), 9)}, Salasnich and Sattin¹⁰⁾. Unfortunately we are not able yet to derive the systematic corrections of higher orders in \hbar expansion to the EBK quantization in more than one dimensional systems. Nevertheless this work helps us to understand the global behaviour and limitations of techniques based on semiclassical ideas. As the higher order corrections yield more accurate results in one dimensional systems we might hope that similar ideas will help to improve the accuracy of the semiclassics in many dimensional cases.

In section 4 we discuss the asymptotic behaviour of exact spectra of nontrivial potentials. By the word nontrivial we mean that the potential in certain range of coordinate possesses a complicated structure, but asymptotically as $|x| \rightarrow \infty$ becomes similar to a simple (scaling) correspondent. We have a strong evidence, exact numerical and semiclassical, that the spectra of both systems do not converge pointwise to the same energy values and not even to a constant energy shift as the energy is increased. Even the convergence of the mean energy level spacing of the two systems is very slow when $E \rightarrow \infty$ (as slow as $E^{-1/4}$).

Appendix A

— Calculation of the zeroth order and the second order terms in the semiclassical quantization formula —

In this section we show how to calculate integrals $\oint d\sigma_0$ and $\oint d\sigma_2$ for the case of asymmetric double-well quartic potential. The integrals that enter the semiclassical quantization condition are calculated separately for the regions where the momentum $p = \sqrt{2(E - V(x))}$ has four and two real zeros.

The contour integrals around the pairs of turning points entering the zeroth and the second order semiclassical formula (2.10) and (2.11) respectively can be written as

$$\oint \sqrt{X} dx = \frac{2}{3} \left[E \oint \frac{dx}{\sqrt{X}} - \frac{\lambda}{4} \oint \frac{x dx}{\sqrt{X}} + \left(1 + \frac{3\lambda^2}{16} \right) \oint \frac{x^2 dx}{\sqrt{X}} \right], \quad (\text{A.1})$$

$$- \oint \frac{X'' dx}{\sqrt{X}} = 12 \left[-\frac{1}{3} \oint \frac{dx}{\sqrt{X}} + \frac{\lambda}{2} \oint \frac{x dx}{\sqrt{X}} + \oint \frac{x^2 dx}{\sqrt{X}} \right]; \quad (\text{A.2})$$

$$X = E - x^4 - \lambda x^3 + 2x^2 = \frac{p^2}{2}.$$

All integrals that we need are

$$I_1 = \oint \frac{dx}{\sqrt{X}}, \quad I_2 = \oint \frac{x dx}{\sqrt{X}}, \quad I_3 = \oint \frac{x^2 dx}{\sqrt{X}}$$

and will be calculated separately for the case where X has four real roots and for the case where X has two real roots.

A.1. Momentum p and X have four real roots ($a < b < c < d$)

The integrals are written for the case of contour integration around a pair of turning points a and b . In case of integration around c and d only substitution

$a \longleftrightarrow c$, $b \longleftrightarrow d$ has to be done.

$$X = E - x^4 - \lambda x^3 + 2x^2 = (x - a)(b - x)(x - c)(x - d)$$

Firstly, we perform a substitution

$$x = \frac{c - dy^2}{1 - y^2}$$

in integrals I_1 , I_2 and I_3 and we get

$$I_1 = \frac{4}{\sqrt{(d-a)(d-b)}} \int_{y_1}^{y_2} \frac{dy}{\sqrt{(y^2 - y_1^2)(y_2^2 - y^2)}} = \frac{4}{\sqrt{(d-a)(d-b)}} J_1;$$

$$y_1 = \sqrt{\frac{b-c}{b-d}}, \quad y_2 = \sqrt{\frac{a-c}{a-d}},$$

$$\begin{aligned} I_2 &= \frac{4}{\sqrt{(d-a)(d-b)}} \left[d \int_{y_1}^{y_2} \frac{dy}{\sqrt{(y^2 - y_1^2)(y_2^2 - y^2)}} - \right. \\ &\quad \left. - (d-c) \int_{y_1}^{y_2} \frac{dy}{(1-y^2)\sqrt{(y^2 - y_1^2)(y_2^2 - y^2)}} \right] = \\ &= \frac{4}{\sqrt{(d-a)(d-b)}} [dJ_1 - (d-c)J_2], \end{aligned}$$

$$\begin{aligned} I_3 &= \frac{4}{\sqrt{(d-a)(d-b)}} \left[d^2 \int_{y_1}^{y_2} \frac{dy}{\sqrt{(y^2 - y_1^2)(y_2^2 - y^2)}} - \right. \\ &\quad \left. - 2d(d-c) \int_{y_1}^{y_2} \frac{dy}{(1-y^2)\sqrt{(y^2 - y_1^2)(y_2^2 - y^2)}} + \right. \\ &\quad \left. + (d-c)^2 \int_{y_1}^{y_2} \frac{dy}{(1-y^2)^2\sqrt{(y^2 - y_1^2)(y_2^2 - y^2)}} \right] = \\ &= \frac{4}{\sqrt{(d-a)(d-b)}} [d^2 J_1 - 2d(d-c)J_2 + (d-c)^2 J_2^{(2)}]. \end{aligned}$$

Factorizing the term $1/(1-y^2)^2$, $J_2^{(2)}$ can be rewritten in the form

$$J_2^{(2)} = \frac{1}{2} J_2 + \frac{1}{4} S,$$

$$S = \int_{y_1}^{y_2} \frac{dy}{(1-y)^2 \sqrt{(y^2 - y_1^2)(y_2^2 - y^2)}} + \int_{y_1}^{y_2} \frac{dy}{(1+y)^2 \sqrt{(y^2 - y_1^2)(y_2^2 - y^2)}}.$$

To calculate S , we use the following relations

$$\begin{aligned} w^2 &= a_0 y^4 + 4a_1 y^3 + 6a_2 y^2 + 4a_3 y + a_4 = \\ &= b_0^{(c)}(y-c)^4 + 4b_1^{(c)}(y-c)^3 + 6b_2^{(c)}(y-c)^2 + 4b_3^{(c)}(y-c) + b_4^{(c)} \end{aligned}$$

and

$$\begin{aligned} b_0^{(c)} \int_{y_1}^{y_2} \frac{(y-c)^2 dy}{w} + 2b_1^{(c)} \int_{y_1}^{y_2} \frac{(y-c) dy}{w} - 2b_3^{(c)} \int_{y_1}^{y_2} \frac{dy}{(y-c)w} &= b_4^{(c)} \int_{y_1}^{y_2} \frac{dy}{(y-c)^2 w}; \\ w(y_1) = w(y_2) &= 0, \quad c \notin (y_1, y_2) \end{aligned} \quad (\text{A.3})$$

(see Magnus *et al*¹¹).

Inserting $w^2 = (y^2 - y_1^2)(y_2^2 - y^2)$ and evaluating the upper expression (A.3) for $c = 1$ and $c = -1$ and subtracting what we get in both cases, we can express S as

$$S = 4 \left[\frac{b_0^{(1)} - 2b_1^{(1)}}{2b_4^{(1)}} J_1 + \frac{b_3^{(1)}}{b_4^{(1)}} J_2 + \frac{b_0^{(1)}}{2b_4^{(1)}} J_3 \right].$$

$$b_0^{(\pm 1)} = -1, \quad b_1^{(\pm 1)} = \mp 1, \quad b_2^{(\pm 1)} = \frac{y_1^2 + y_2^2}{6} - 1,$$

$$b_3^{(\pm 1)} = \pm \left(\frac{y_1^2 + y_2^2}{2} - 1 \right), \quad b_4^{(\pm 1)} = (y_1^2 + y_2^2) - y_1^2 y_2^2 - 1.$$

Integrals

$$J_1 = \frac{1}{y_2} \mathbf{F}(m), \quad J_2 = \frac{1}{y_2} \mathbf{F}(m) + \frac{y_1^2}{y_2(1 - y_1^2)} \mathbf{\Pi}(n, m), \quad J_3 = y_2 \mathbf{E}(m),$$

$$m = \frac{y_2^2 - y_1^2}{y_2^2}, \quad n = \frac{m}{1 - y_1^2}$$

can be found in (Gradshteyn *et al*¹²) or (Abramowitz and Stegun¹³). Functions $\mathbf{F}(m)$, $\mathbf{E}(m)$ and $\mathbf{\Pi}(k, m)$ are the complete elliptic integrals of the first, the second and the third kind as defined by Abramowitz and Stegun.

Finally we can write

$$\begin{aligned} \oint d\sigma_0 &= \frac{8\sqrt{2}}{3} \frac{1}{\sqrt{(d-b)(c-a)}} \\ &\left\{ \left[E - \frac{1}{2} \left(1 + \frac{3\lambda^2}{16} \right) (cd + ab) - \frac{3c\lambda}{4} \left(1 + \frac{\lambda^2}{8} \right) \right] \mathbf{F}(m) + \right. \\ &\quad + \frac{1}{2} \left(1 + \frac{3\lambda^2}{16} \right) (d-b)(c-a) \mathbf{E}(m) + \\ &\quad \left. + \frac{3\lambda}{4} \left(1 + \frac{\lambda^2}{8} \right) (c-b) \mathbf{\Pi}(n, m) \right\}; \end{aligned} \quad (\text{A.4})$$

$$m = \frac{(d-c)(b-a)}{(c-a)(d-b)}, \quad n = \frac{b-a}{c-a},$$

and

$$\oint d\sigma_2 = -\frac{1}{\sqrt{2}} \frac{\partial}{\partial E} \frac{1}{\sqrt{(d-b)(c-a)}} \left\{ \left(cd + ab + \frac{2}{3} \right) \mathbf{F}(m) - (d-b)(c-a) \mathbf{E}(m) \right\}. \quad (\text{A.5})$$

A.2. *Momentum p and X have two real roots ($a_1 < a_2$, $b \pm ci$)*

$$X = E - x^4 - \lambda x^3 + 2x^2 = (x - a_1)(a_2 - x)((x - b)^2 + c^2)$$

In this case the substitution

$$x = \frac{a_2 + a_1 \frac{q}{k} \tan^2 \frac{\phi}{2}}{1 + \frac{q}{k} \tan^2 \frac{\phi}{2}};$$

$$k^2 = (a_1 - b)^2 + c^2, \quad q^2 = (a_2 - b)^2 + c^2$$

is performed in integrals I_1 , I_2 and I_3 and following the similar procedure as in the case of 4 real roots of X , the integrals can be rewritten in the following form

$$I_1 = \frac{4}{\sqrt{kq}} \mathbf{F}(m);$$

$$m = \frac{kq - (a_1 - b)(a_2 - b) - c^2}{2kq}, \quad n = -\frac{(k - q)^2}{4kq},$$

$$I_2 = \frac{4}{\sqrt{kq}} \left[\frac{a_2 k - a_1 q}{k - q} \mathbf{F}(m) - \frac{(a_2 - a_1)k + q}{2} \frac{k + q}{k - q} \mathbf{\Pi}(n, m) \right],$$

$$I_3 = \frac{4}{\sqrt{kq}} \left[\frac{a_2^2 k - a_1^2 q}{k - q} \mathbf{F}(m) + kq \mathbf{E}(m) - (a_1 + a_2 + 2b) \frac{(a_2 - a_1)k + q}{4} \frac{k + q}{k - q} \mathbf{\Pi}(n, m) \right].$$

By using these expressions, $\oint d\sigma_0$ and $\oint d\sigma_2$ can be finally written as

$$\begin{aligned} \oint d\sigma_0 = \frac{8\sqrt{2}}{3} \frac{1}{\sqrt{kq}} & \left\{ \left[E - \frac{\lambda}{4} \frac{a_2 k - a_1 q}{k - q} + \left(1 + \frac{3\lambda^2}{16} \right) \frac{a_2^2 k - a_1^2 q}{k - q} \right] \mathbf{F}(m) + \right. \\ & + \left(1 + \frac{3\lambda^2}{16} \right) kq \mathbf{E}(m) + \\ & \left. + \frac{3\lambda}{8} \left(1 + \frac{\lambda^2}{8} \right) \frac{(a_2 - a_1)(k + q)}{k - q} \mathbf{\Pi}(n, m) \right\}; \quad (\text{A.6}) \end{aligned}$$

$$k^2 = (a_1 - b)^2 + c^2, \quad q^2 = (a_2 - b)^2 + c^2,$$

$$m = \frac{kq - (a_1 - b)(a_2 - b) - c^2}{2kq}, \quad n = -\frac{(k - q)^2}{4kq}.$$

and

$$\oint d\sigma_2 = \frac{1}{\sqrt{2}} \frac{\partial}{\partial E} \frac{1}{\sqrt{kq}} \left\{ \left(2 \frac{a_2^2 k - a_1^2 q}{k - q} + \lambda \frac{a_2 k - a_1 q}{k - q} - \frac{2}{3} \right) \mathbf{F}(m) + 2kq \mathbf{E}(m) \right\}. \quad (\text{A.7})$$

In the section 4 we use the generalized form of the asymmetric quartic potential

$$V(x) = x^4 + \mu(\lambda x^3 - 2x^2) \Rightarrow X = E - x^4 - \lambda \mu x^3 + 2\mu x^2 = \frac{p^2}{2}.$$

In this case the integral (A.1) is slightly modified to

$$\oint \sqrt{X} dx = \frac{2}{3} \left[E \oint \frac{dx}{\sqrt{X}} - \mu \frac{\lambda \mu}{4} \oint \frac{x dx}{\sqrt{X}} + \left(\mu + \frac{3(\lambda \mu)^2}{16} \right) \oint \frac{x^2 dx}{\sqrt{X}} \right], \quad (\text{A.8})$$

yielding the μ dependent expression (4.13) for σ_0 , which is identical to (A.6) for $\mu = 1$. Please note that the parameters k , q , m , n as well as the integrals I_1 , I_2 and I_3 are expressed in terms of the four roots of X and momentum and so is their general dependence on μ already considered.

Appendix B
 ——— Some tables of results ———

Table I. Some eigenenergies of the homogeneous quartic potential. By n we denote the consecutive quantum number of the state, while E_{Exact} is the exact energy value of the eigenstate, and $E_{Semi}^{(0)}$, $E_{Semi}^{(2)}$, and $E_{Semi}^{(4)}$ are the semiclassically predicted energy eigenvalues of the n th state, calculated with the zeroth order, second order and the fourth order semiclassical quantization formula.

n	E_{Exact}	$E_{Semi}^{(0)}$	$E_{Semi}^{(2)}$	$E_{Semi}^{(4)}$
0	0.6679862591	0.5462673250	0.6178440470	0.5994975436
	5577710827	7809440985	9454695175	8186297455
1	2.3936440164	2.3635614446	2.4003574561	2.3991273384
	8230311603	0057710124	2199197003	3857621598
2	4.6967953868	4.6705199316	4.6968569596	4.6965336443
	6364619622	9480733314	9157646544	2176087907
3	7.3357299952	7.3148026019	7.3358836919	7.3357508981
	2709279884	0083816986	7629989381	3385710476
4	10.2443084554	10.2265364336	10.2443782077	10.2443100572
	3877107597	1101923867	8948408161	3952052722
...
100	643.1833913927	643.1811392054	643.1833914100	643.1833913927
	8056430848	7609028834	9319827383	8185826816
101	651.7305795719	651.7283422013	651.7305795888	651.7305795719
	7519147803	2623003831	3668259301	7642701540
103	668.9091219363	668.9069134812	668.9091219523	668.9091219363
	1714901544	9348071280	2366319599	1827702401
105	686.1986791466	686.1964986907	686.1986791618	686.1986791466
	2251646322	3792741559	3254876433	2354809723
...
495	5397.2204747691	5397.2196972873	5397.2204747693	5397.2204747691
	2444635012	4414211246	7029195001	2444710621
496	5411.7486521189	5411.7478756815	5411.7486521192	5411.7486521189
	9592537080	1512620174	4045276381	9592611981
497	5426.2865864811	5426.2858110844	5426.2865864813	5426.2865864811
	2223840485	4128681921	6545729016	2223914687
500	5469.9588010681	5469.9580287730	5469.9588010683	5469.9588010681
	5121968046	5845185750	9057033639	5122040195
...
1000	13774.2520020553	13774.2515153776	13774.2520020553	13774.2520020553
	0377443322	5917115936	4151998141	0377446170
1005	13866.1108150810	13866.1103300181	13866.1108150811	13866.1108150810
	7240132753	5261252080	0964842617	7240135535
1008	13921.2992811341	13921.2987970336	13921.2992811341	13921.2992811341
	4444693588	5119763791	8139930100	4444696331
1009	13939.7076086294	13939.7071248487	13939.7076086295	13939.7076086294
	9093649576	4694282718	2779132907	9093652307
1010	13958.1220154946	13958.1215320331	13958.1220154946	13958.1220154946
	3736333880	1516055405	7412099391	3736336599

Table II. Some eigenenergies of the asymmetric double-well quartic potential with $\hbar_{eff} = 1$, $\lambda = 0.2$, ($\mu = 1$). By n we denote the consecutive quantum number of the state, while E_{Exact} are the exact energy value of the n th eigenstate and $E_{Semi}^{(2)}$ are the semiclassically predicted energy eigenvalues of the n th state, calculated with the second order semiclassical quantization formula.

n	E_{Exact}	$E_{Semi}^{(2)}$
0	-0.17296458264338966970	-0.1733140474651558
1	0.65867088851932470219	0.7915823554184969
2	2.51962151763406920996	2.501600214006679
3	4.63865676589239143594	4.640576944608262
...
100	619.636315269976695643	619.6363152899056
101	628.028868586785663262	628.0288686061785
103	644.899655331227155754	644.8996553496056
105	661.883432587416475526	661.8834326048518
...
495	5329.38195574207411204	5329.381955742333
496	5343.81915399412485822	5343.819153994382
497	5358.26617031658854323	5358.266170316844
500	5401.66599550160242755	5401.665995501854

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